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Investigation of the characteristic properties of high-order harmonic spectrum in atoms using Bohmian trajectories

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Abstract
We study the electron quantum dynamics of high harmonic generation (HHG) processes of atomic hydrogen under intense near infrared (NIR) laser fields by means of the De Broglie–Bohm’s framework of Bohmian mechanics. The proposed accurate 3D numerical scheme is utilized to discuss the mechanism of the multiple plateau generation and the cut-off extension, as the main characteristic features of HHG spectrum. One-color (1600 nm) and two-color (1600 nm + 800 nm) laser fields with different time delays are used to investigate the effect of pulse shape on electron dynamics and HHG process. The presented results on Bohmian trajectories and their energy content, along with the analysis of the emission time period of different groups of trajectories, provide a comprehensive and fresh electron dynamical picture and uncover novel mechanisms of the HHG processes and power spectra.

Keywords: high harmonic generation, Bohmian mechanics, electron dynamics

(Some figures may appear in colour only in the online journal)
One approach to Bohmian mechanics is the hydrodynamics formation of quantum mechanics, in which the probability amplitude and the phase of the wave function are transported along the quantum trajectories and observables may be computed directly in terms of this information. In the de Broglie-Bohm, on the other hand, the individual tracer particles are evolved along quantum trajectories with the velocities generated by the time-dependent wave function field. The patterns developed by these quantum trajectories as they emerge from an ensemble of initial points exactly define the history of the system as it evolves from the initial to final state. This allows one to employ de Broglie–Bohm’s framework of Bohmian mechanics (BM) to provide an accurate trajectory-based scheme to interpret the electron wave packet dynamics [21].

Bohmian mechanics has been applied to investigate a variety of phenomena such as photo-dissociation [23], tunneling [24], atom diffraction by surface [25], etc., in the past. More recently, it has been also used to model the study of strong field processes such as HHG [26], laser-driven electron dynamics [27–34], etc. However, most of the BM studies of strong field processes so far have adopted either 1D or soft-potential models. We recently proposed a fully ab initio three-dimensional and accurate treatment of the Bohmian trajectories beyond SFA, and utilized it to explore the sub-cycle multi-photon ionization dynamics of hydrogen atom subject to intense near infrared (NIR) laser fields on the sub-femtosecond time scale [35].

The formation of several plateaus in the HHG spectrum in the process of interaction of a gas with two-color laser pulses has been studied previously [36–38]. In this paper, we investigate the electron dynamical mechanism of high harmonic generation by analyzing the Bohmian trajectories. We treat the interaction of an intense laser field with a single hydrogen atom by solving the time-dependent Schrödinger equation (TDSE); atomic units are used:

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \psi(r, t) = \left[ \hat{H}_0 + \hat{V}(r, t) \right] \psi(r, t),
\]

where \( \hat{H}_0 \) is the unperturbed Hamiltonian of the hydrogen atom and \( \hat{V}(r, t) \) is the time-dependent interaction of the electron with the laser field in the dipole approximation:

\[
\hat{V}(r, t) = -F(t) \hat{r} = -zeF(t),
\]

\( F(t) \) being the force acting upon the electron from the laser field. The general form of the laser pulse is formulated (for one- and two-color fields) by

\[
F(t) = A_1 f_1(t) \sin(\omega_1 t + \phi_1) + A_2 f_2(t - \tau) \times \sin(\omega_2(t - \tau) + \phi_2),
\]

where \( A_1 \) and \( A_2 \) are the peak field amplitudes, \( \omega_1 \) and \( \omega_2 \) are the carrier frequencies, \( f_1(t) \) and \( f_2(t - \tau) \) are the Gaussian envelopes, \( \tau \) is the time delay between both mid-infrared laser pulses, and \( \phi_1 \) and \( \phi_2 \) are the carrier-envelope phases (CEP), which are both set as zero. Without loss of generality, we can assume that the polarization vector of the field lies in \( z \)-direction. The carrier wavelengths are \( \lambda_1 = 1600 \text{ nm (} \omega_1 = 0.028 \text{ a.u.}) \) and \( \lambda_2 = 800 \text{ nm (} \omega_2 = 0.057 \text{ a.u.}) \), and the peak intensities are \( A_1 = 3.5 \times 10^{13} \text{ W cm}^{-2} \) and \( A_2 = 0.8 \times 10^{13} \text{ W cm}^{-2} \). The duration of the Gaussian pulses are 8 and 5 fs, respectively. We consider electron dynamics under a single color laser and two cases of two-color lasers with \( \tau = 0.5 T_2 \) and \( \tau = 1.0 T_2 \) \( (T_2 = \frac{2\pi}{\omega_2}) \).

The time-dependent generalized pseudo-spectral (TDGPS) method [39] is used to solve the TDSE in spherical coordinates accurately and efficiently. This method takes advantage of the generalized pseudo-spectral (GPS) technique for non-uniform optimal spatial discretization of the coordinates and the Hamiltonian using only a modest number of grid points. The time propagation of the wave function under this method is performed by the split operator method in the energy representation [39]. To impose correct outgoing-wave boundary conditions on the wave function and prevent spurious reflections from the boundary of the spatial domain, we use an absorbing layer at large distances from the atomic core. The absorber is implemented through the mask function \( \cos^{0.25}(\pi \left( r - r_0 \right)/2(r_{max} - r_0)) \), \( r \geq r_0 \) with \( r_{max} = 100 \text{ a.u.}, r_0 = 80 \text{ a.u.} \). The wave function is multiplied by the mask function at each time step. Because of the absorber, the norm of the wave function decreases in time.

The expectation value of the dipole acceleration, is obtained from the time-dependent wave function:

\[
d_A(t) = |\langle \psi(r, t) | \frac{e^z}{r} + F(t) | \psi(r, t) \rangle|.
\]

The corresponding HHG power spectrum from a hydrogen atom exposed to the laser field is obtained, in the single-atom level, by the Fourier transformation of time-dependent dipole acceleration as follows:

\[
P_A(\omega) = \left| \frac{1}{T_f - T_i} \omega^2 \int_{T_i}^{T_f} d_A(t) e^{-i\omega t} \right|^2.
\]

where \( \omega \) is the fundamental frequency, \( \omega = 0.028 \text{ a.u. (} \lambda = 1600 \text{ nm).} \)

The detailed spectral and temporal time-dependent structure of HHG can be investigated by performing the wavelet spectrum as the following [40],

\[
A(t, \omega) = \int \sqrt{\omega} d_A(t') W(\omega(t' - t)) dt'
\]

Here \( W(\omega(t' - t)) \) is the mother wavelet. For the harmonic emission, a natural choice of mother wavelet is given by the Morlet wavelet [40],

\[
W(\chi) = \frac{1}{\sqrt{\pi}} e^{i\chi} e^{-\chi^2/2\tau^2}.
\]

For atoms in linearly polarized laser fields, the angular momentum projection onto the polarization direction of the field (the \( z \)-axis) is conserved. That means the dependence of the wave function on the angle \( \varphi \) (rotation angle about the \( z \)-axis) is reduced to the factor \( \exp(\text{i} m \varphi) \), where \( m \) is the angular momentum projection. For \( m = 0 \) the wave function
does not depend on $\varphi$ at all. Let us consider a tracer particle co-moving with the quantum probability density flow. The velocity of such a particle is calculated from the quantum-mechanical current density $j$ and probability density, $\rho$ as $\mathbf{v} = j/\rho$ where $\rho = |\psi|^2$. and $j = 1/2i(\psi^* \nabla \psi - \psi \nabla \psi^*)$. Then the path of this particle, that is the Bohmian trajectory, can be obtained by solving the following equation:

$$\frac{dr}{dt} = \text{Im}(\frac{\nabla \psi}{\psi}).$$

(8)

The first step for Bohmian mechanics calculations is to obtain the time-dependent wave function by solving the TDSE equation, equation (1). Then the gradient of the wave function, $\psi(r, t)$, can be calculated with respect to the coordinates $r$ (radial coordinate) and $\theta$ (angle between the radius-vector and z-axis):

$$\nabla \psi = e_r \frac{\partial \psi}{\partial r} + e_{\theta} \frac{\partial \psi}{\partial \theta} - e_{\theta} \sin \theta \frac{\partial \psi}{\partial r} - e_{\theta} \cos \theta \frac{\partial \psi}{\partial \theta}.$$  

(9)

e_r and $e_{\theta}$ are the unit vectors of spherical coordinate system. Since the velocity $\frac{dr}{dt}$ has the following expansion in the spherical coordinate system,

$$\frac{dr}{dt} = e_r \frac{dr}{dt} + e_{\theta} \frac{d\theta}{dt} + e_{\varphi} \sin \theta \frac{d\varphi}{dt},$$

the vector equation (8) is equivalent to a set of three 1D equations:

$$\frac{dr}{dt} = \text{Im} \left( \frac{1}{\psi} \frac{\partial \psi}{\partial r} \right).$$

(11)

$$\frac{d\theta}{dt} = -\frac{\sin \theta}{r^2} \text{Im} \left( \frac{1}{\psi} \frac{\partial \psi}{\partial \cos \theta} \right).$$

(12)

$$\frac{d\varphi}{dt} = 0.$$  

(13)

Obviously, the angle $\varphi$ does not change, and the trajectory lies in the plane defined by the initial (at $t = t_0$) radius-vector and the z-axis. One has to solve the Cauchy problem for the set of two equations (11) and (12). In the generalized pseudo-spectral (GPS) discretization, we use the Gauss–Lobatto scheme for the variable $r$ (with the appropriate mapping transformation) and the Gauss scheme for the variable $\cos \theta$. The expression for the first derivative with respect to $r$ appears as follows [41–43]:

$$\left( \frac{\partial \psi}{\partial r} \right)_{(r,s)} = \frac{1}{r^2(s)} \sum_{j=1}^{N_r} P_{N+1}(s_j) \int_{r_0}^{r} d\psi \psi \left( x_j \right).$$

(14)

Here, $P_{N+1}$ is the Legendre polynomial. $N_r$ is the number of collocation points (roots of the derivative of Legendre polynomial, $P_{N+1}^{\prime}$(x)), not including the end points -1 and +1. The matrix elements for the $d_{y^j}^y$ Gauss–Lobatto discretization are as listed below:

$$d_{y_j}^y = \frac{1}{x_j - x_j}, \quad d_{y_j}^j = 0 \quad (j \neq j'),$$

$$d_{y_N}^j = -\frac{N(N+1)}{4}, \quad d_{y_N}^N = \frac{N(N+1)}{4}.$$  

(15)

The first derivative with respect to $\cos \theta$ is as follows:

$$\left( \frac{\partial \psi}{\partial \cos \theta} \right)_{cos \theta} = \sum_{j=1}^{N_r} P_{N+1}(y_j) \int_{cos \theta} d\psi \psi \left( \left( \cos \theta_j \right) \right).$$

(16)

Here $N_r$ is the number of collocation points in the Gauss scheme (roots of the Legendre polynomial $P_{N+1}$). Equation (15) assumes that the mapping transformation is just the identity transformation, i.e. $\cos \theta = y$. The matrix elements $d_{y^y}^y$ are defined as following:

$$d_{y_j}^y = \frac{1}{y_j - y_j}, \quad d_{y_j}^j = \frac{y_j}{1 - y_j^2}. \quad (j \neq j'),$$

(17)

To calculate the first derivative of the Legendre polynomials, one can use the following recursion relation:

$$P_{N+1}^\prime(y) = \frac{N(N+1)}{2N+1} \left[ P_{N-1}(y) - P_{N+1}(y) \right].$$

(18)

The set of coupled ordinary differential equations (11) and (12) is solved numerically with the help of the 4th order Runge–Kutta (RK4) method, yielding the electron quantum trajectories. Since the quadrature points for RK4 differ from the original GPS grid points, we need to perform an additional interpolation using the GPS interpolation formula [35, 43], to be able to evaluate the numerical values of the wave function at the coordinate points supplied by the RK4 solver:

$$\psi(r, \theta, t) = \sum_{i=1}^{N_r} \sum_{j=1}^{N_r} \psi(r_i, \theta_j, t) \frac{P_{N+1}(x_i)}{(2N+3)(x_i - x_j)P_{N+1}(x_i)} \times \left[ \frac{P_{N}(y)}{(P_{N-1}(y) - P_{N+1}(y))} \right].$$

(19)

In this study, since the laser fields are linearly polarized in z-direction, the initial conditions are chosen to be $x_0 = 1$ and $1 \leq z_0 \leq 10$ (in atomic units). Although the proposed method is robust and is not sensitive to the selected initial conditions, we found that this set best represents the dynamics of electron under the given laser fields. As demonstrated in [35] one can also take the advantage of electron density analysis to gain a clear insight on choosing the best initial conditions under different circumstances.
In figure 1 we explore the effect of modifying the pulse shape and see its consequence on the HHG power spectrum. The results presented in this figure are acceleration from the power spectra of a hydrogen atom exposed to each of the three given laser fields. In each case the ionization and emission time intervals are obtained from Bohmian mechanics calculations and illustrated on the laser field plots in figures 1(a), (c), (e). Here, we only study the dynamics of the wave packets which detach, travel under external laser field and return to the parent ion within the two central optical cycles (−0.5 through 1.5 o.c.). This is because the contribution of the travelling wave packets in the other time intervals are found to be very low (due to lower laser field intensity) to the HHG generation.

In figures 1(a), (c), (e), the red shaded areas, labeled (1) and (1’), indicate the first detachment and return time, respectively. Similarly, the green shaded areas, labeled (2) and (2’), indicate the second detachment and return time, respectively. The position of the bumps in the pulse shape due to the time delays are shown by letters ‘A’, ‘B’, and ‘C’. On each HHG spectrum, the range of the plateau is given.

**Figure 1.** Driving laser fields $F(t)$, and the corresponding HHG power spectra for hydrogen atom for ((a), (b)) fundamental frequency laser field, ((c), (d)) Two-color laser field with time delay of $\tau = 0.5 T_o$, and ((e), (f)) Two-color laser field with time delay of $\tau = 1.0 T_o$. On each laser field plot, the red shaded areas, labeled (1) and (1’), indicate the first detachment and return time, respectively. Similarly, the green shaded areas, labeled (2) and (2’), indicate the second detachment and return time, respectively. The position of the bumps in the pulse shape due to the time delays are shown by letters ‘A’, ‘B’, and ‘C’. On each HHG spectrum, the range of the plateau is given.
generates another plateau with higher intensity not only extends the cut-off for about 10 harmonics, but also this power spectrum applying the other two-color laser which is more smooth and synchronized. The result of higher intensity signal, broader and smoother super-con-tribution of different groups of trajectories in electron dynamics under each of these laser fields, to inves-tigate the contribution of different groups of trajectories in electron dynamics under each of these laser fields.

The commonly used tool to investigate the HHG process is the strong-field approximation (SFA). However, the SFA is based on several approximations, including (a) negligible ionization of the ground state, (b) dropping the Coulomb potential and treating only the ground and the (free-particle) continuum states, and (c) limitation to the weak or medium strong monochromatic laser fields [44]. In the De Broglie–Bohm’s framework of the Bohmian mechanics, however, quantum electron trajectories are directly obtained from accurate quantum mechanical treatment of the system under investigation, and therefore both the time-dependent laser field and the binding potential are fully incorporated. Next, we will analyze the Bohmian trajectories, which represent the electron dynamics under each of these laser fields, to inves-tigate the contribution of different groups of trajectories in generation of variety range of high harmonics.

Bohmian trajectories provide a detailed perspective on the evolution of quantum electron density. The distinct Bohmian trajectories represent the evolution of the travelling wave packets in space and time, and therefore properly illustrate their contributions into the harmonic spectrum [35]. In figure 2 the Bohmian trajectories illustrate the electron dynamics within the few central optical cycles, when each of the given laser fields are at their highest intensities. As represented by these trajectories, following the direction of the force from the laser field, first a distinct and uniform density packet is shaped and detached from the atom and moves toward the negative z-direction. A big portion of these trajectories (pink) returns back to the parent ion when the force from the laser field becomes positive. As indicated by the dotted red line, the first ionized front wave travels to \(-90 < Z_{\text{max}} < -80\) before it changes direction and returns to the core. The duration of this return is different in each case. As indicated on each plot, the electron trajectories under the two-color laser field with a time delay of \(\tau = 1.0T_z\), figure 1(c), has the most extended first return time, about 0.55 o.c. Next, would be the single-color laser, figure 1(a), with the first return occurring in an approximately 0.45 o.c. time interval. On the other hand, one can see that although the first return in figure 1(b) occurs in the smallest time period, about 0.3 o.c., however this two color laser field with the time delay of \(\tau = 0.5T_z\) has the highest second return time duration, about 0.5 o.c.

To be able to discuss the main features of the HHG spectrum for each case, we first need to analyze the effect of time delay to explain the observations we just made on the return time intervals, and also provide a qualitative picture for the travelling wave packets under each of the given laser fields. When the fundamental laser field is applied to the hydrogen atom, figure 1(a), after \(-0.5\) o.c., a single portion of electron density detached from the core towards the negative z-direction. Besides the outer-most part of this detached electron density that leaves the core after some oscillations in the external laser field (gray out-going trajectories), some detached wave packets return to the parent ion when the force from the laser field becomes positive [35]. The pink trajectories in figure 2(b) (bottom panel) represent the dynamics of this group of electron density. When the laser electric field changes sign, these ‘pink’ trajectories change direction and travel back to the core. The return process happens in a time interval of about 0.45 o.c. As we will be discussing later in this paper, since the returning trajectories travel different distances before they return to the core, each of them would have different return energies. This causes transitions to excite bound and continuum states over time. As indicated in figures 1(a), (e), and as one can also clearly see in figures 2(a), (c), the first return (1') and the second ionization (2) completely overlap. In other words, the second ionization toward positive z-direction, (green trajectories, labeled by (2)), starts while some portions of wave packets are still returning from the negative z-direction, (1'). The oscillations of the electron density at the core due to this ongoing return process results in generation of multiple wave packets, instead of just one, for the second ionization [35, 45]. Therefore second ionization toward positive z-direction happens as several relatively distinct density portions detach from the core. The situation is different when we apply the two color laser field with the time delay of \(\tau = 0.5T_z\), figure 1(c). This time delay in the laser field, makes two bumps in the pulse shape (indicated by ‘A’ and ‘B’). The first bump, ‘A’, is placed when the first ionization process (1), is happening. This effectively postpones the first return process (1'), so that, as one can clearly see in figure 2(b), the overlap between the first return (1') and the second ionization (2) is minimized. The effect of this separation is pronounced in the quality of the second detached electron trajectories. In the absence of the oscillations from the first return process, a more uniform portion of electron
In all three studied cases, due to higher laser intensities, some portions of the detached densities at this step can be directly ionized and do not return to the core (immediately out-going gray trajectories). Some trajectories, however, return to the parent ion (green) when the force from the laser field change the sign. As indicated by a dash green line, in each case the maximum distance that these wave packets travel before they return is smaller ($Z_{\text{max}} < 50$). The emission time periods ($2'$), for each case are given in figure 2 as well. A clear expansion of the return time (about 0.5 o.c.) for the case of the two color laser field with the time delay of $\tau = 0.5T_2$, can be justified by the existence of the second bump in the pulse shape (indicated by 'B'). Since this bump is positioned when the second return ($2'$) is occurring, it gives the process more time, thus resulting in extended emission time for this laser field. The same argument can be made for the case of the two color laser field with the time delay of $\tau = 1.0T_2$. Here, the time delay makes a bump (indicated by

Figure 2. Bohmian trajectories illustrating the dynamics of electron wave packets travelling toward negative (lower panel; pink) and positive (upper panel; green) $z$-direction. For each case, several trajectories (colored solid lines) are selected as representatives for different groups of trajectories to analyze their energy contributions in HHG. Labels (1) and (1') indicate the first detachment and return time, respectively. Similarly, labels (2) and (2') indicate the second detachment and return time, respectively. The ionization and return time intervals are also given for each process. The presented results are for (a) fundamental frequency laser field, (b) Two-color laser field with time delay of $\tau = 0.5T_2$, and (c) Two-color laser field with time delay of $\tau = 1.0T_2$. 
during the first return process (‘1’), which, as expected, gives more time for the electron wave packets to return and therefore results in an extended emission time (about 0.55 o.c.).

To correlate these findings to the structural characteristics in the corresponding HHG spectrum, several trajectories (colored solid lines) are selected as representatives for different groups of trajectories. The evolution of the electron energy with time for these selected trajectories will be discussed in detail to analyze their contribution in HHG.

Figure 3 shows the evolution of the electron energy in some of the individual trajectories selected in figure 2. The energy is calculated as $E_k + E_p$, where $E_k$ and $E_p$ are the kinetic and Coulomb potential energies, respectively. Several prominent features are observed.

(a) For each laser field, the left travelling trajectories (lower panels in figure 2) contribute to higher harmonics. This can be explained by the fact that preceding returning trajectories in this group experience a longer distance ($-90 < Z_{max} < -80$) and therefore gain more energy under the influence of the external laser field. The energy contributions of the right traveling trajectories (upper panels in figure 2), on the other hand, are limited to the lower harmonics, due to the fact that these groups of trajectories travel shorter distance ($50 < Z_{max} < 65$) under the external laser field. The energy profiles of the representative trajectories shown in figures 3(b1) and (b2), clearly illustrate this remark for the case of the two-color laser field with time delay of $\tau = 0.5T_2$. For the other two cases, namely the fundamental laser field, figure 3(a), and the two-color laser field with time delay of $\tau = 1.0T_2$, figure 3(c), we found that the dominant contribution in HHG is from the left traveling wave packets. As explained above, this is because of the disturbance effect of the first return on the second ionization, which, in turn, results in fewer numbers of trajectories with synchronized emission time for each harmonic.

(b) The electron dynamical origin of the multiple plateau generation can also be discussed by using the here presented results. The two color laser field with $\tau = 0.5T_2$ which generates more intense and uniform portions of electron densities during both first and second ionization process, figure 2(b), provides two plateaus in the HHG spectrum, figure 1(d). The correspondence between the energy content of the Bohmian trajectories and the two HHG plateaus demonstrates that the

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**Figure 3.** The evolution of the electron energy with time for some of the selected trajectories (see figure 2) obtained from Bohmian calculations. The presented results are for (a) Left-traveling trajectories under the fundamental frequency laser field, corresponding to the lower panel in figure 2(a). (b1) Right-traveling trajectories under the two-color laser field with time delay of $\tau = 0.5T_2$ corresponding to the upper panel in figure 2(b). (b2) Left-traveling trajectories under the two-color laser field with time delay of $\tau = 0.5T_2$ corresponding to the lower panel in figure 2(b). (c) Left-traveling trajectories under the two-color laser field with time delay of $\tau = 1.0T_2$, corresponding to the lower panel in figure 2(c).
Figure 4. HHG power spectra for the wave packets traveling toward positive z-direction (upper panel) and negative z-direction (lower panel). For each case the contributions to the time frequency wavelet profiles (right panels) are presented as well. The results are for (a) fundamental frequency laser field, (b) two-color laser field with time delay of $\tau = 0.5T$, and (c) two-color laser field with time delay of $\tau = 1.0T$. On each HHG spectrum, the range of plateau is given. The red and green arrows indicate the emission peaks due to return of the negative z-direction and positive z-direction raveling wave packets, respectively.
first returning wave packets (pink) are more responsible for the generation of the second plateau, and the second returning wave packets (green) are dominantly contribute in the formation of the first plateau in figure 1(d).

(c) Also, the expansion of the plateaus for different laser fields is found to be related to the return time period of the corresponding group(s) of trajectories. For instance, one can see that the two color laser field with the time delay of \( \tau = 1.07T \), figure 1(e) has more expanded plateau, compared to the other two lasers. As presented in figure 2(c), this is because of the extension of the first return time period, to about 0.55 o.c. On the other hand, as illustrated in figure 3(c), the corresponding time profile and energy evolution of the wave packets under this laser field show relatively concentrated emission time of the short-trajectory electrons, compared to the rather broad and dispersive emission time of the short-trajectory electrons travelling under the fundamental laser field, figure 3(a).

The information provided by Bohmian mechanics about the individual trajectories, \( Z_t(t) \), and their energy content, along with the analysis of the emission time period of these groups of trajectories provide a comprehensive and intuitive picture of the HHG process. As we will show next, this causal interpretation can serve in complement to the results obtained from direct analysis of the expectation value of the induced dipole moment, \( \langle Z \rangle = \langle \psi(r, t) | Z | \psi(r, t) \rangle \). Therefore, at the next step, we will use the TDSE results to further discuss these findings and to provide an unambiguous proof for the mechanism we proposed.

Based on the knowledge we obtained from analyzing the Bohmian results about the energy contribution of different groups of electron trajectories during the two ionization/return processes, we propose a unique approach to explore the TDSE results in order to confirm our above findings. Since the Bohmian trajectories, figure 2, show a split between the left and right \((-z\) and \(+z\) directions respectively) travelling wave packets, we separate the time-dependent wave function during TDSE propagation into two portions, and investigate the contribution of each of them in harmonic generation. Taking this numerical step allows us to check the validity of the conclusions we made on the contributions of different groups of trajectories in harmonic generation and the role of pulse shape in the structure of the HHG spectrum.

Each of the left panels of figure 4 show the HHG power spectra generated from only the right travelling (upper panel) and the left travelling (lower panel) TDSE wave function. The main feature of this result is that for each given laser field we have been able to find the dominant contributing wave packets in harmonic generations. To do so, one should compare the separated HHG power spectra in figure 4 with the total ones provided in figure 1. As shown in figure 3, the left traveling wave packets contribute to higher harmonics. In complement to Bohmian mechanics results presented in figure 3, this phenomenon is clearly seen in figure 4 as well.
For the case of the two color laser field with the time delay of $t = T_0.5$, comparison between figures 1(d) and 4(b) proves that the first plateau, H18-H36, is formed due the second return process, labeled (2') in figure 2(b), while the second plateau, H44-H60, is mainly generated from the first return, labeled (1') in figure 2(b).

The corresponding wavelet time-frequency profiles are also presented for each case for the separated wave packets at the right panels. This is considered as unambiguous evidence of the existence of the Bremsstrahlung radiation which is emitted by the re-collision of the electron wave packet with the parent ionic core. In each presented profile, the darker red color indicates that a higher population of electron trajectories are contributing to the generation of those particular harmonics. The effect of laser pulse manipulation, by using different time delays, on the expansion of the emission time is clearly shown in here presented wavelet profiles. For each case, the red and green arrows show the dominant peak.

Figure 5 presents the dipole time profiles of the consecutive harmonics within an optical cycle obtained from TDSE calculations. The resemblance between the energy patterns presented in figure 3 and the time profiles are well pronounced for all the cases. Both data indicate that short and long trajectories are contributing in generation of the harmonics in the plateaus. For instance, the energy patterns in figure 3(c) and the time profiles in figure 5(c), both, indicate that the short trajectories fall into two more synchronized groups to emit the illustrated consecutive harmonics.

In summary, we presented fully ab initio scheme to accurately investigate the electron dynamics during the HHG process within the De Broglie–Bohm’s framework of Bohmian mechanics. The detachment of electron wave packets from a hydrogen atom under a fundamental NIR laser field and a couple of different two-color laser fields were analyzed. The presented Bohmian trajectories and their energy profiles, along with the corresponding HHG power spectra and wavelet time-frequency profiles, were discussed to explore the formation of multiple plateau and cut-off extension during HHG process. The method presented is quite general and can also be extended to the study of more complex atomic and molecular systems. We believe that this causal interpretation
of quantum mechanics by Bohmian mechanics is a necessary and complementary approach to the recent development of the real-time experimental observation of ultrafast electron dynamics in atomic and molecular systems. This technique will allow us to design better driving lasers for different applications by providing an accurate tool to better monitor and control the electron dynamics.

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